Androst-1,4-dien-17«beta»-methyl-17«alpha»-ol-3-one TMS

InChI: InChI=1S/C26H44O2Si2/c1-24-15-12-20(27-29(4,5)6)18-19(24)10-11-21-22(24)13-16-25(7)23(21)14-17-26(25)28-30(8,9)31

InchiKey: BSSYZSWTKYGGLG-URDCWPSYSA-N

Formula: C26H44O2Si2

SMILES: CC12C=CC(O[Si](C)(C)C)=CC1=CCC1C2CCC2(C)C1CCC2(C)O[Si](C)(C)C

Mol. weight [g/mol]: 444.80

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.52		Crippen Method
logp	7.681		Crippen Method
rinpol	2668.00		NIST Webbook
rinpol	2684.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R321912&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices